Detection of Pair-Superfluidity for bosonic mixtures in optical lattices

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We consider a mixture of two bosonic species with tunable interspecies interaction in a periodic potential and discuss the advantages of low filling factors on the detection of the pair-superfluid phase. We show how the emergence of such a phase can be put dramatically into evidence by looking at the interference pictures and density correlations after expansion and by changing the interspecies interaction from attractive to repulsive.

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Ultra-cold atoms in optical lattices are presently one of the best environments for the study of exotic quantum phases [1, 2]. The experimental demonstration of the superfluid to Mott transition [3] has opened the way to the study of strongly correlated phases in lattices. In the case of mixtures of different atomic species or different internal levels, new phenomena related to quantum magnetisms and spin physics arise [4].

The quantum phase that is central to this work is the pair-superfluid (PSF) phase for a mixture of two different bosonic species. This phase consists in the formation of a superfluid of pairs where atoms of different species preferentially hop together in the lattice. It is characterised by the vanishing of the single-species order parameter and by the emergence of a pair-order parameter. This problem is related to the historical question formulated, e.g., by Nozières and Saint James [5], concerning the impossibility of coexistence of single and pair superfluidity. This impossibility lies in the fact that a single species condensate is associated with the macroscopic occupation of the zero momentum (quasi-momentum) state for each species, while a pair superfluid requires the macroscopic occupation of the zero relative momentum, without any constraint on the value that the single species momenta can separately take. As a consequence, single species condensation is destroyed. In this work, we will see how this picture is directly reflected into physical quantities accessible in experiments.

The existence of a pair-superfluid phase in lattices has been already pointed out in several papers [6, 7, 8, 9, 10, 11, 12, 13]. The main emphasis has been put on the situation of equal density for the two species leading to total integer and half integer filling factor. For integer filling factors, PSF arises in the regime where the interspecies interaction almost completely compensates the repulsive intraspecies interaction. Unfortunately, the precision on the values of the interaction strengths and the very small values of the tunneling parameter required to get pair superfluidity, makes this phase almost unaccessible experimentally. At half filling factor for each species (total integer filling), the PSF phase (analogous to the $x-y$ ferromagnet) is predicted in a larger region of the phase space. At low tunneling and in the presence of asymmetries between the interaction and tunneling parameters of the two species, the PSF phase competes with the insulating-like anti-ferromagnetic ordering. Instead for total incommensurate filling factor, no insulating-like phases (Mott or antiferromagnetic-like) exist. In this regime, easily accessible signatures for the experimental observation of pair superfluidity are available. In this paper, we would like to complement the predictions in [13], discussing the role played by the two-body momentum distribution and commenting on the effect of interactions in the expansion.

At total incommensurate filling factor and zero temperature, two important phases are naturally conceived [14]: (i) a double superfluid (2SF), where both species are independently superfluid and single-species coherence exists, and (ii) a PSF phase, characterized by pair coherence. Assuming that interactions do not affect significantly the expansion of the atomic cloud after release, all required information needed to distinguish between the two phases are included in the pictures of the two species after expansion: first of all, the interference fringes, typical of single-species coherence, will appear for the 2SF phase and vanish in the case of PSF. Moreover, the density-density correlations between the two species after expansion carry information about the correlations in momentum space before expansion, which are dramatically different for the two phases.

We consider two bosonic atomic species in a lattice, described by the Bose-Hubbard Hamiltonian

$$\begin{aligned} H \;=\; & -\sum_{\langle ij\rangle}\left[J_a a_i^\dagger a_j + J_b b_i^\dagger b_j\right] + \\ & +\sum_{i,\sigma}\left[\frac{U_\sigma}{2} n_i^\sigma (n_i^\sigma - 1)\right] + \sum_i U_{ab} n_i^a n_i^b, \end{aligned} \tag{1}$$

where $\sigma = a, b$ indicates the two bosonic species, $a_i, b_i, a_i^\dagger, b_i^\dagger$, and n_i^σ are respectively the annihilation, creation operators and the density of species a and b at site i. The notation $\langle ij\rangle$ represents nearest neighbors. The intraspecies on-site interactions U_σ and tunneling parameters J_σ depends in the standard way on the optical lattice potential and scattering lengths. Generally speaking the most favorable conditions for PSF are given by a complete symmetry between the two species, as far as interaction, hopping and density are concerned. This is the situation that we will assume in this paper ($N_a = N_b = N$,

$J_a = J_b = J$, $U_a = U_b = U$), focusing on the possibility of changing the interspecies interaction U_{ab} from negative to positive by tuning the interspecies scattering length via a Feshbach resonance over a wide range, as demonstrated in [15].

The solution of Hamiltonian (1) is a non-trivial many-body task. Quantum Monte Carlo (QMC) calculations provide the most accurate results [6, 8, 10]. Evidences of the PSF phase have been recently obtained also by matrix-product-state [9, 12, 13] and dynamical mean-field approaches [11]. Instead the standard mean-field approximation based on a generalized Gutzwiller Ansatz $|\Phi\rangle = \prod_i \sum_{n,m} f^{(i)}_{n,m} |n_a, n_b\rangle_i$, which in principle includes correlations between the two atomic species, misses the pair superfluid phase due to the impossibility of correctly accounting for second order hopping which is at the origin of the PSF phase. Recently, a treatment based on a mean-field analysis of the effective Hamiltonian in the pair-subspace applied to a bilayer system of 2D dipolar lattice bosons has proven successful to describe the PSF and pair-supersolid (PSS) phases [17].

In order to capture the basic physics of the pair correlations underlying the emergence of the PSF, in this work we employ a toy-model based on the exact diagonalisation of (1) for a system of few atoms occupying few lattice wells in 1D with periodic boundary conditions. Of course sharp phase transitions are not accounted for by our treatment, but we believe that the main conclusions remain valid also for larger systems and higher dimensions.

The comparison between filling factor equal to and less than 1/2 is useful, since for filling factor exactly equal to 1/2, there exist a particle-hole symmetry between positive and negative interspecies interaction in the almost hard-core limit $|U_{ab}| \ll U$, leading to the pairsuperfluid phase (PSF) for attractive interactions (pairing of two atoms of different species) and the so-called countersuperfluid phase (SCF) for repulsive interactions (pairing of one atom with a hole of the other species). Instead, for equal filling factor less than 1/2 for each species, PSF still persist, but SCF pairing is suppressed. This different behaviour for positive and negative interspecies interaction might help identifying the formation of PSF as discussed below.

In order to put into evidence the differences between filling factor $\nu = 1/2$ and $\nu < 1/2$, we will consider a system of 4 wells and 2 atoms of each species ($N_w = 4$, $N = 2$) and a system of 6 wells and 2 atoms of each species ($N_w = 6$, $N = 2$), which are the smallest cases including the possibility of having equal filling factors $\nu \leq 1/2$ and non trivial on-site interactions. We look at the following quantities [16]:

$$\mathcal{V}_{2SF} = \langle a_i^\dagger a_{i+1} \rangle = \langle b_i^\dagger b_{i+1} \rangle, \tag{2}$$

$$\mathcal{V}_{PSF} = \langle a_i^\dagger b_i^\dagger a_{i+1} b_{i+1} \rangle - \langle a_i^\dagger a_{i+1} \rangle \langle b_i^\dagger b_{i+1} \rangle, \tag{3}$$

$$\mathcal{V}_{SCF} = \langle a_i^\dagger b_i a_{i+1} b_{i+1}^\dagger \rangle - \langle a_i^\dagger a_{i+1} \rangle \langle b_i b_{i+1}^\dagger \rangle. \tag{4}$$

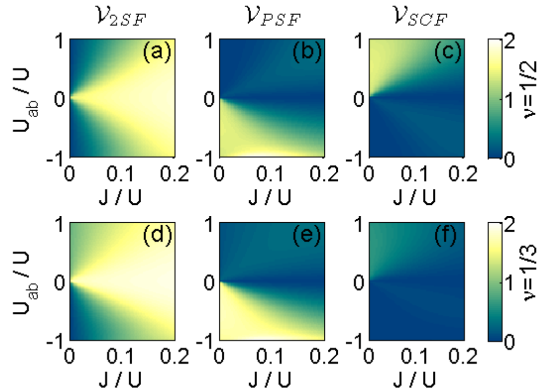

FIG. 1: (Color online) Phase diagram for $N_w = 4, 6$ (upper and lower row, respectively) and $N = 2$. (a,d) Single-particle coherence $N_w \mathcal{V}_{2SF}$, as defined in Eq.(2); (b,e) Pair coherence $N_w \mathcal{V}_{PSF}$, as defined in Eq.(3); (c,f) Counter-pair coherence $N_w \mathcal{V}_{SCF}$, as defined in Eq.(4). The factor N_w allows a better comparison between the two different lattice sizes. The region of parameters of strong attractive interaction $U_{ab} < -U$ corresponds to collapse in a large system.

The quantities $\mathcal{V}_{2SF}$, $\mathcal{V}_{PSF}$ and $\mathcal{V}_{CSF}$ characterise respectively the 2SF, PSF and SCF phases. We also consider single particle and two-particle momentum distributions in order to make a useful link to the experiments.

In Fig.1, we show the phase diagram as a function of J and U_{ab}. One can clearly identify the PSF (or SCF) regions as the dark regions in Fig.1(a,d) where single-species coherence vanishes, and at the same time pair-coherence (or counter-pair coherence) is different from zero, namely the light regions in Fig.1(b,e) (or Fig.1(c) for SCF). As explained above, for $\nu = 1/2$, PSF and SCF are found respectively for attractive and repulsive interaction. Instead, for $\nu < 1/2$, SCF is absent. For low filling, the crossover from 2SF to PSF is governed by the competition between the single particle hopping J and the energy cost for breaking a pair, equal to $|U_{ab}|$. For that reason, PSF is found for attractive interspecies interactions at sufficiently low tunneling parameter $J \ll |U_{ab}|$.

An important quantity accessible in experiments, which would provide an unquestionable proof of PSF, is the measure of correlations in the momentum distribution, reflecting the fact that in the PSF and SCF phases, two atoms of different species form a pair and condense in the state of total quasi-momentum $q_a \pm q_b = 0$ (respectively for atom-atom and atom-hole pairs), as shown in Fig.2(a,c,f). In the case of two non interacting superfluids ($U_{ab} = 0$), the two species have completely uncorrelated momentum distributions, i.e. $n^{(a,b)}(q_a, q_b) = n^{(a)}(q_a) \times n^{(b)}(q_b)$, where $n^{(a)}(q_a)$ and $n^{(b)}(q_b)$ separately present interference peaks at even multiples of the Bragg momentum q_B (see Fig.2(b,e)), as happens for standard single component condensates [3, 18]. In the presence of interspecies interactions $U_{ab} \neq 0$, correlations build up

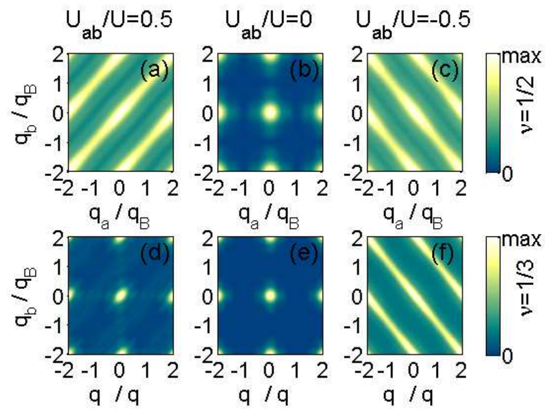

FIG. 2: (Color online) Two-body momentum distribution $n^{(a,b)}(q_a, q_b)$ for $N = 2$ and $N_w = 4, 6$, i.e. filling factor 1/2 and 1/3 (upper and lower row, respectively). (a,d) repulsive interparticle interaction $U_{ab} = 0.5U$; (b,e) vanishing interparticle interaction $U_{ab} = 0$; (c,f) attractive interparticle interaction $U_{ab} = -0.5U$. In all pictures $J = 0.01U$. Two Brillouin zones are shown for clarity.

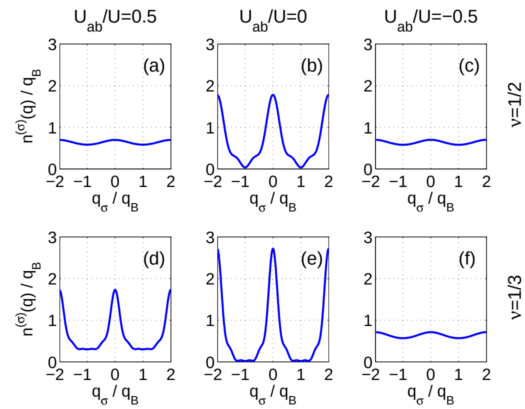

FIG. 3: Single species momentum distribution $n^{(\sigma)}(q_\sigma)$ for $N = 2$ and $N_w = 4, 6$, i.e. filling factor 1/2 and 1/3 (upper and lower row, respectively). (a,d) repulsive interparticle interaction $U_{ab} = 0.5U$; (b,e) vanishing interparticle interaction $U_{ab} = 0$; (c,f) attractive interparticle interaction $U_{ab} = -0.5U$. In all pictures $J = 0.01U$. Two Brillouin zones are shown for clarity.

in a very different way depending on the filling factor and on whether the interactions are repulsive or attractive. For filling factors exactly equal to 1/2, the situation is almost symmetric for positive and negative U_{ab} upon particle-hole duality for the different species. The momentum correlations are opposite in the two cases, as shown in Fig.2(a,c), showing SCF and PSF respectively. The 2SF phase is recovered in the vicinity of vanishing interspecies interactions (Fig.2(b)). For equal filling factor smaller than 1/2, a 2SF is obtained both for vanishing and repulsive interactions (Fig.2(d,e)), since the filling factor of one species does not match the filling factor of the holes of the other. Hence, only negligible momentum correlations exist for $U_{ab} \geq 0$. On the contrary, attractive interactions lead to PSF and very strongly correlate the two different species ($U_{ab}/U = -0.5$, Fig.2(f)).

The correlations in the two-body momentum distribution are strictly related to single-particle coherence and strongly affect the visibility of the single particle momentum distribution, as shown in Fig. 3. The presence of momentum correlations in $n^{(a,b)}(q_a, q_b)$ lead to a reduced contrast in $n^{(\sigma)}(q_\sigma)$. Hence, some signatures of the formations of the PSF/SCF phases are provided already by the interference in the single-particle expansion pictures, which is the most easily accessible experimental method [13]. For instance, at low enough tunneling, for $\nu < 1/2$ interference is expected at $U_{ab} \geq 0$, while it disappears (under exactly the same conditions) by tuning U_{ab} to negative values.

Most important, the single species expansion pictures carry information about the momentum correlations. In fact, as demonstrated in [19], the direct measurement of the momentum correlations can be performed by looking at the noise in the single-species expansion pictures [20, 21]. Assuming first that interactions do not affect the expansion, the single-species densities after time of flight are given by $n^{\sigma}_{\rm TOF}(r_\sigma = q_\sigma t/m_\sigma) = n^{(\sigma)}(q_\sigma)$. Hence, in the case of PSF, where the correlations are of the type $q_a + q_b = 0$, we expect the two expansion pictures to be correlated at correctly rescaled opposite positions and possibly at corresponding points in different Brillouin zones.

In usual experiments, interatomic interactions are not turned off during the expansion, and their effect is considered to be negligible due to the higher energy scales involved in the problem. In the present case, it would be a safe procedure to tune at least U_{ab} to zero just before releasing the cloud. However, this might not be so easily achievable in an experiment. For this reason, we have performed simple numerical estimations of the effect of the interspecies interactions on the expansion for two atoms released from a 4-well lattice (see Fig.4). While the effect of relatively weak attractive interactions ($|U_{ab}|/J \approx 20$, see Fig.4(a,b)), the two-body momentum distribution is hardly modified during the expansion, we have seen that the two-body momentum distribution can be affected by attractive interspecies interaction U_{ab}, for interaction strengths leading to pairing ($|U_{ab}|/J \approx 60$, see Fig.4(c,d)). This effect tends to create also some correlations along the diagonal $q_a = q_b$, but does not destroy the correlations typical of the PSF phase (at $q_a = -q_b$). Hence, recovering the two-body density after expansion via noise correlation measurements, the distinction between PSF and 2SF phases still remains very clear. More dramatic effects of the interactions during the expansion take place only for values of $|U_{ab}|/J$ which are much beyond the estimated onset of the PSF phase transition.

Small asymmetries in the Hamiltonian parameters of the two species do not destroy the PSF phase. Instead, an unbalance in the densities of atoms a and b hinders the

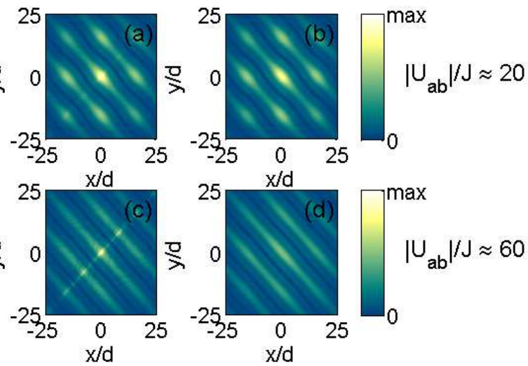

FIG. 4: (Color online) Effect of attractive interspecies interaction U_{ab} on the expansion. (a,c) Two-body density after expansion after a time of flight $E_r t_{\mathrm{TOF}} \approx 12$, where E_r is the recoil energy, in the presence of interspecies interaction U_{ab}; (b,d) Free expansion at the same time of flight (shown for comparison). The strengths of interaction are $|U_{ab}|/J \approx 20$ in (a,b) and $|U_{ab}|/J \approx 60$ in (c,d) respectively.

formation of the pairs. Unfortunately, we are not able to quantify the realistic effect of the unbalance due to the small number of atoms considered. However, one can think of experimental procedures to create a sample with almost exactly equal populations of the two species. For instance, one could start with a Mott insulator at unit filling for both species, and then tailor the optical potentials, introducing a second laser at half the wavelength, such to split each lattice well into two equal ones. Applying this procedure along two dimensions would lead to a filling factor of exactly 1/4 for each species. This procedure should remain valid also in the presence of an external harmonic confinement, especially in the case of very low tunneling, where the central Mott region at unitary filling is dominant with respect to the outer superfluid shell. Alternatively, one can create a unitary filled Mott region for both species in the trap center and then release the harmonic trap till the desired filling factor is reached. This method would favor the creation of the pairs in the Mott phase, which can then become superfluid once the filling factor is made incommensurate.

The physical ingredient on which pair superfluidity relies is the second order hopping of two atoms of the different species at once. This is closely related to the exchange interaction, whose observability has been recently demonstrated in [22]. The fact that pair hopping is a second order process in J, where J is assumed to be small, might seem to be discouraging for the experimental observation of the PSF phase. However, exact QMC simulations of this problem [10], in line with the results of our toy-model, predict the transition between 2SF and PSF, at half integer filling and symmetry between the two species, to happen at $J \approx 0.1\,|U_{ab}|$. Exploiting the possibility of having U_{ab} of the same order of U, this leads to relatively large values for the critical tunneling. On the other hand, careful analysis about the critical temperature and entropy for the formation of the PSF phase, as recently done in [23], are required.

Our model provides an oversimplified description of the system. We believe however that it includes correctly the fundamental ingredients of the physics involved. A more quantitative analysis based on exact numerical calculations, including the effects of two-species unbalance on the formation of the paired phases, will be subject of future work.

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